Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 06:33 AM EDT

PDB ID	:	5X3T
Title	:	VapBC from Mycobacterium tuberculosis
Authors	:	Kang, S.M.; Kim, D.H.; Yoon, H.J.; Lee, B.J.
Deposited on	:	2017-02-07
Resolution	:	2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

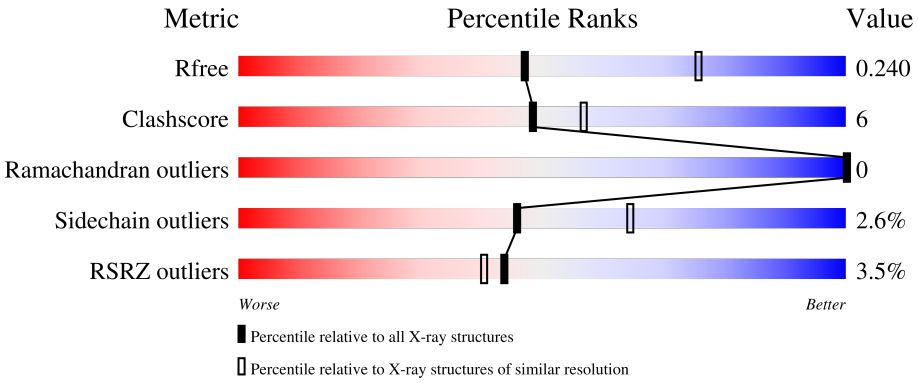
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



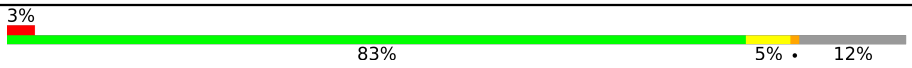
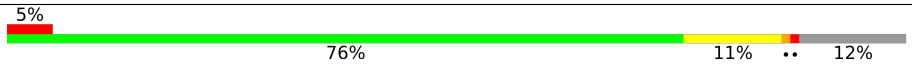
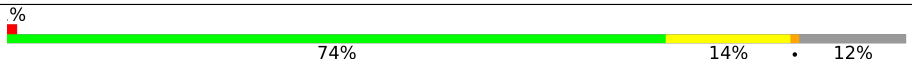
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	71	90% 7% ••
1	C	71	3% 79% 18% ••
1	E	71	10% 52% 32% • 14%
1	G	71	8% 58% 25% • 14%
2	B	155	84% • • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	155	
2	F	155	
2	H	155	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6169 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Antitoxin VapB26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	70	Total	C	N	O	Se	0	0	0
			523	324	100	97	2			
1	C	70	Total	C	N	O	Se	0	0	0
			523	324	100	97	2			
1	E	61	Total	C	N	O	Se	0	0	0
			457	282	91	82	2			
1	G	61	Total	C	N	O	Se	0	0	0
			457	282	91	82	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MSE	LEU	engineered mutation	UNP O53778
C	50	MSE	LEU	engineered mutation	UNP O53778
E	50	MSE	LEU	engineered mutation	UNP O53778
G	50	MSE	LEU	engineered mutation	UNP O53778

- Molecule 2 is a protein called Ribonuclease VapC26.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	137	Total	C	N	O	S	Se	0	0	0
			1036	651	183	199	2	1			
2	D	137	Total	C	N	O	S	Se	0	0	0
			1036	651	183	199	2	1			
2	F	137	Total	C	N	O	S	Se	0	0	0
			1036	651	183	199	2	1			
2	H	137	Total	C	N	O	S	Se	0	0	0
			1036	651	183	199	2	1			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MSE	-	expression tag	UNP O53779
B	-18	GLY	-	expression tag	UNP O53779
B	-17	SER	-	expression tag	UNP O53779
B	-16	SER	-	expression tag	UNP O53779
B	-15	HIS	-	expression tag	UNP O53779
B	-14	HIS	-	expression tag	UNP O53779
B	-13	HIS	-	expression tag	UNP O53779
B	-12	HIS	-	expression tag	UNP O53779
B	-11	HIS	-	expression tag	UNP O53779
B	-10	HIS	-	expression tag	UNP O53779
B	-9	SER	-	expression tag	UNP O53779
B	-8	SER	-	expression tag	UNP O53779
B	-7	GLY	-	expression tag	UNP O53779
B	-6	LEU	-	expression tag	UNP O53779
B	-5	VAL	-	expression tag	UNP O53779
B	-4	PRO	-	expression tag	UNP O53779
B	-3	ARG	-	expression tag	UNP O53779
B	-2	GLY	-	expression tag	UNP O53779
B	-1	SER	-	expression tag	UNP O53779
B	0	HIS	-	expression tag	UNP O53779
D	-19	MSE	-	expression tag	UNP O53779
D	-18	GLY	-	expression tag	UNP O53779
D	-17	SER	-	expression tag	UNP O53779
D	-16	SER	-	expression tag	UNP O53779
D	-15	HIS	-	expression tag	UNP O53779
D	-14	HIS	-	expression tag	UNP O53779
D	-13	HIS	-	expression tag	UNP O53779
D	-12	HIS	-	expression tag	UNP O53779
D	-11	HIS	-	expression tag	UNP O53779
D	-10	HIS	-	expression tag	UNP O53779
D	-9	SER	-	expression tag	UNP O53779
D	-8	SER	-	expression tag	UNP O53779
D	-7	GLY	-	expression tag	UNP O53779
D	-6	LEU	-	expression tag	UNP O53779
D	-5	VAL	-	expression tag	UNP O53779
D	-4	PRO	-	expression tag	UNP O53779
D	-3	ARG	-	expression tag	UNP O53779
D	-2	GLY	-	expression tag	UNP O53779
D	-1	SER	-	expression tag	UNP O53779
D	0	HIS	-	expression tag	UNP O53779
F	-19	MSE	-	expression tag	UNP O53779
F	-18	GLY	-	expression tag	UNP O53779
F	-17	SER	-	expression tag	UNP O53779

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-16	SER	-	expression tag	UNP O53779
F	-15	HIS	-	expression tag	UNP O53779
F	-14	HIS	-	expression tag	UNP O53779
F	-13	HIS	-	expression tag	UNP O53779
F	-12	HIS	-	expression tag	UNP O53779
F	-11	HIS	-	expression tag	UNP O53779
F	-10	HIS	-	expression tag	UNP O53779
F	-9	SER	-	expression tag	UNP O53779
F	-8	SER	-	expression tag	UNP O53779
F	-7	GLY	-	expression tag	UNP O53779
F	-6	LEU	-	expression tag	UNP O53779
F	-5	VAL	-	expression tag	UNP O53779
F	-4	PRO	-	expression tag	UNP O53779
F	-3	ARG	-	expression tag	UNP O53779
F	-2	GLY	-	expression tag	UNP O53779
F	-1	SER	-	expression tag	UNP O53779
F	0	HIS	-	expression tag	UNP O53779
H	-19	MSE	-	expression tag	UNP O53779
H	-18	GLY	-	expression tag	UNP O53779
H	-17	SER	-	expression tag	UNP O53779
H	-16	SER	-	expression tag	UNP O53779
H	-15	HIS	-	expression tag	UNP O53779
H	-14	HIS	-	expression tag	UNP O53779
H	-13	HIS	-	expression tag	UNP O53779
H	-12	HIS	-	expression tag	UNP O53779
H	-11	HIS	-	expression tag	UNP O53779
H	-10	HIS	-	expression tag	UNP O53779
H	-9	SER	-	expression tag	UNP O53779
H	-8	SER	-	expression tag	UNP O53779
H	-7	GLY	-	expression tag	UNP O53779
H	-6	LEU	-	expression tag	UNP O53779
H	-5	VAL	-	expression tag	UNP O53779
H	-4	PRO	-	expression tag	UNP O53779
H	-3	ARG	-	expression tag	UNP O53779
H	-2	GLY	-	expression tag	UNP O53779
H	-1	SER	-	expression tag	UNP O53779
H	0	HIS	-	expression tag	UNP O53779

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Mg 1 1	0	0

- Molecule 4 is water.

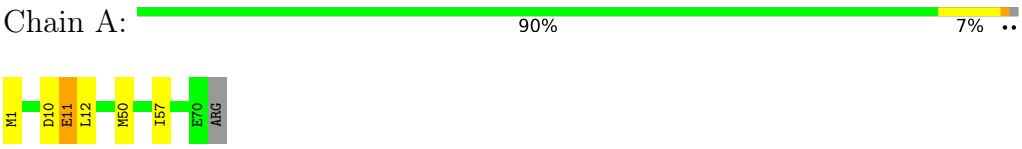
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	C	6	Total O 6 6	0	0
4	E	4	Total O 4 4	0	0
4	B	17	Total O 17 17	0	0
4	D	9	Total O 9 9	0	0
4	F	12	Total O 12 12	0	0
4	H	13	Total O 13 13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

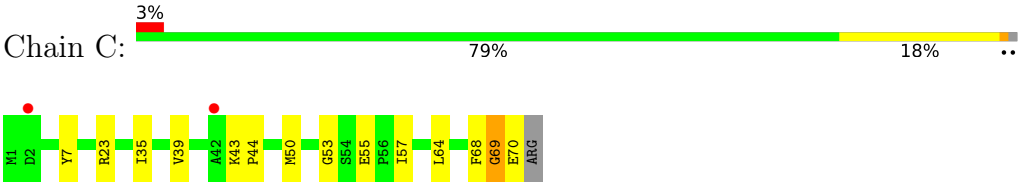
• Molecule 1: Antitoxin VapB26

Chain A:



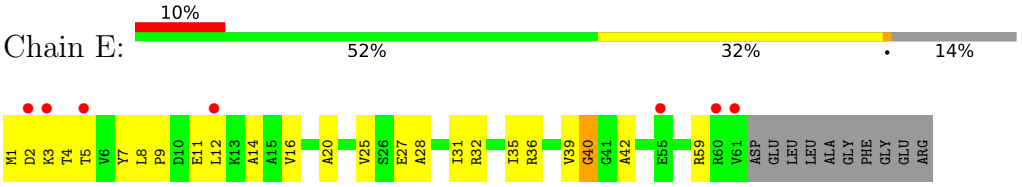
• Molecule 1: Antitoxin VapB26

Chain C:



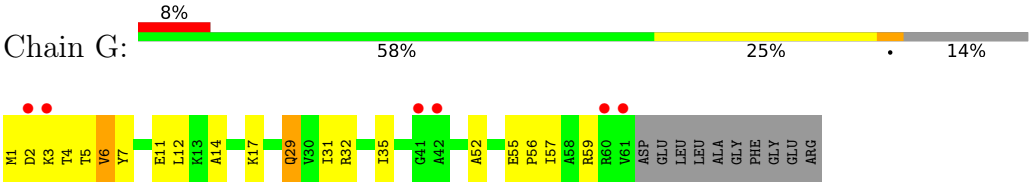
• Molecule 1: Antitoxin VapB26

Chain E:



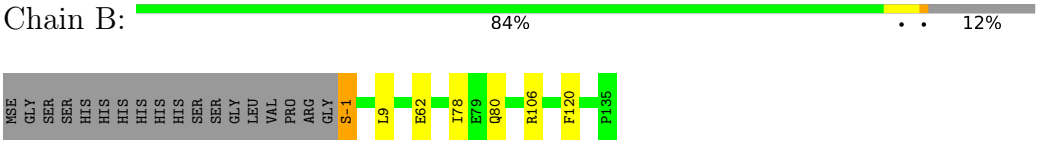
• Molecule 1: Antitoxin VapB26

Chain G:



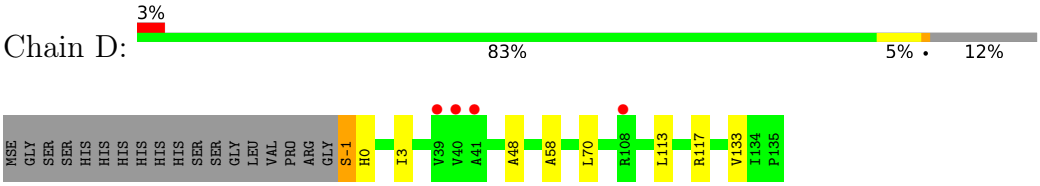
• Molecule 2: Ribonuclease VapC26

Chain B:



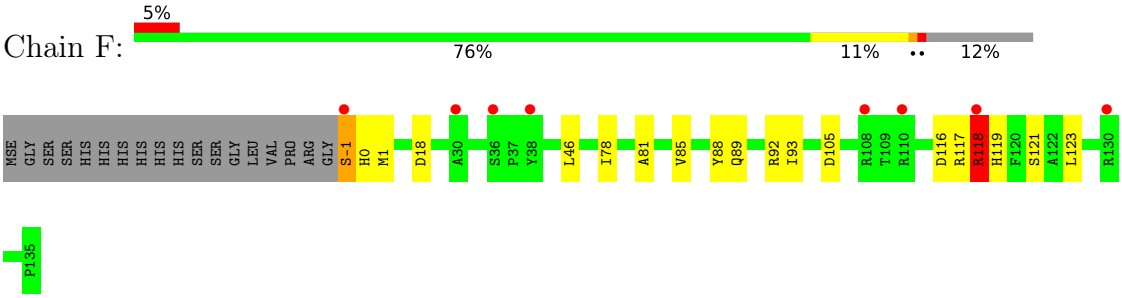
• Molecule 2: Ribonuclease VapC26

Chain D:



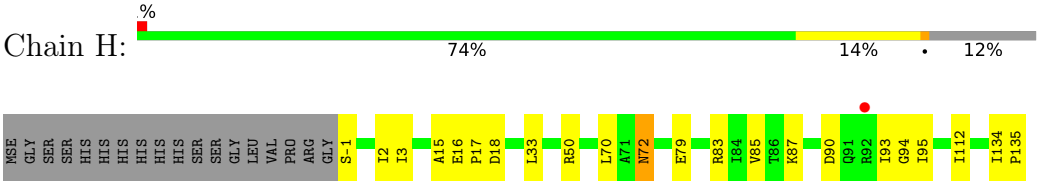
• Molecule 2: Ribonuclease VapC26

Chain F:



• Molecule 2: Ribonuclease VapC26

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	64.22Å 64.22Å 216.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.78 – 2.65 29.33 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.78-2.65) 98.0 (29.33-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 2.26Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.239 0.216 , 0.240	Depositor DCC
R_{free} test set	1967 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6169	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/529	0.55	0/709
1	C	0.33	0/529	0.61	1/709 (0.1%)
1	E	0.39	0/462	0.76	1/619 (0.2%)
1	G	0.34	0/462	0.60	0/619
2	B	0.33	0/1051	0.51	0/1431
2	D	0.32	0/1051	0.53	0/1431
2	F	0.37	0/1051	0.64	0/1431
2	H	0.32	0/1051	0.53	0/1431
All	All	0.33	0/6186	0.58	2/8380 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	1
2	F	0	3
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	40	GLY	N-CA-C	7.01	130.62	113.10
1	C	69	GLY	N-CA-C	5.91	127.88	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	53	GLY	Peptide
1	C	68	PHE	Peptide
1	E	39	VAL	Peptide
2	F	118	ARG	Peptide
2	F	88	TYR	Peptide
2	F	89	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	523	0	541	6	0
1	C	523	0	541	9	0
1	E	457	0	483	20	0
1	G	457	0	483	20	0
2	B	1036	0	1034	7	0
2	D	1036	0	1034	7	0
2	F	1036	0	1034	12	0
2	H	1036	0	1034	19	0
3	H	1	0	0	0	0
4	A	3	0	0	0	0
4	B	17	0	0	1	0
4	C	6	0	0	0	0
4	D	9	0	0	0	0
4	E	4	0	0	0	0
4	F	12	0	0	1	0
4	H	13	0	0	0	0
All	All	6169	0	6184	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:ALA:HB1	2:F:92:ARG:HH22	1.30	0.93
2:F:-1:SER:O	2:F:0:HIS:ND1	2.06	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:THR:HG22	1:G:3:LYS:HG2	1.65	0.78
2:H:79:GLU:OE2	2:H:83:ARG:NH1	2.21	0.73
1:E:2:ASP:OD2	1:G:7:TYR:HA	1.88	0.72
2:B:-1:SER:HA	4:B:214:HOH:O	1.96	0.66
2:H:85:VAL:HA	2:H:93:ILE:HD11	1.79	0.64
2:H:93:ILE:HG13	2:H:94:GLY:H	1.63	0.64
2:F:118:ARG:HA	2:F:121:SER:H	1.63	0.63
1:A:50:MSE:HE1	2:B:62:GLU:HB2	1.81	0.62
1:A:11:GLU:HG3	1:A:12:LEU:H	1.67	0.59
1:G:59:ARG:NH1	2:H:18:ASP:OD2	2.36	0.58
1:G:55:GLU:HG2	1:G:56:PRO:HD2	1.86	0.58
2:H:16:GLU:HG3	2:H:17:PRO:HD2	1.86	0.58
1:G:57:ILE:HG21	2:H:50:ARG:CD	2.34	0.57
1:E:59:ARG:NH1	2:F:18:ASP:OD1	2.38	0.56
1:E:5:THR:HA	1:G:4:THR:O	2.05	0.55
1:E:35:ILE:HD11	1:G:31:ILE:HG23	1.89	0.54
1:C:69:GLY:O	2:F:46:LEU:HD11	2.08	0.54
1:A:11:GLU:HG3	1:A:12:LEU:N	2.23	0.53
2:H:3:ILE:HD11	2:H:33:LEU:HB3	1.91	0.52
1:E:8:LEU:HB3	1:E:12:LEU:HD11	1.91	0.52
2:D:70:LEU:HD13	2:F:78:ILE:HD12	1.91	0.52
2:F:118:ARG:HB2	2:F:121:SER:HB2	1.92	0.51
1:G:57:ILE:HG21	2:H:50:ARG:HD2	1.92	0.50
2:B:80:GLN:HE22	2:B:106:ARG:HH12	1.60	0.50
1:E:42:ALA:N	1:G:11:GLU:OE2	2.41	0.50
2:H:134:ILE:HB	2:H:135:PRO:HD2	1.93	0.49
1:G:57:ILE:HG21	2:H:50:ARG:HD3	1.94	0.49
2:B:80:GLN:NE2	2:B:106:ARG:HH12	2.11	0.49
1:E:9:PRO:HB2	1:E:11:GLU:OE1	2.14	0.48
2:F:85:VAL:HA	2:F:93:ILE:HD11	1.96	0.48
1:A:57:ILE:HD11	2:B:9:LEU:HD22	1.95	0.48
2:F:93:ILE:HG21	2:F:123:LEU:HD21	1.96	0.47
1:G:1:MSE:HG3	1:G:2:ASP:N	2.28	0.47
2:H:93:ILE:HG13	2:H:94:GLY:N	2.28	0.47
1:C:57:ILE:HG22	1:C:64:LEU:HD22	1.97	0.47
2:D:3:ILE:HG23	2:D:113:LEU:HD23	1.97	0.47
1:E:3:LYS:HD2	1:E:3:LYS:N	2.30	0.47
1:G:59:ARG:HD2	2:H:18:ASP:OD1	2.14	0.46
2:F:81:ALA:O	2:F:85:VAL:HG23	2.15	0.46
1:C:69:GLY:HA2	1:C:70:GLU:HA	1.42	0.45
1:G:14:ALA:HA	1:G:17:LYS:HE2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASP:OD1	1:A:11:GLU:N	2.49	0.45
1:E:7:TYR:HE2	1:G:2:ASP:HB3	1.81	0.45
1:E:28:ALA:O	1:E:32:ARG:HG3	2.15	0.45
2:D:117:ARG:HG3	2:D:133:VAL:HG11	1.98	0.45
1:G:29:GLN:HA	1:G:32:ARG:HB2	1.97	0.45
1:E:36:ARG:HA	1:E:40:GLY:HA3	1.99	0.44
2:F:1:MSE:HG2	4:F:204:HOH:O	2.17	0.44
1:E:31:ILE:HD12	1:G:6:VAL:HG11	2.00	0.44
1:A:1:MSE:HE3	1:C:7:TYR:HB3	1.99	0.44
1:E:11:GLU:O	1:E:14:ALA:HB3	2.18	0.44
2:D:-1:SER:O	2:D:0:HIS:CG	2.70	0.44
2:H:2:ILE:HB	2:H:112:ILE:HD13	1.99	0.44
1:E:16:VAL:CG1	1:E:27:GLU:HB2	2.48	0.44
1:C:43:LYS:HA	1:C:44:PRO:HD3	1.70	0.43
1:E:2:ASP:OD1	1:E:2:ASP:C	2.56	0.43
2:B:78:ILE:HD12	2:H:70:LEU:HD13	2.00	0.43
2:H:95:ILE:HD12	2:H:95:ILE:HA	1.87	0.43
1:E:4:THR:O	1:G:5:THR:HA	2.18	0.43
1:C:55:GLU:O	1:C:55:GLU:HG3	2.19	0.43
2:H:87:LYS:HE3	2:H:87:LYS:HB2	1.90	0.42
1:E:59:ARG:NH2	2:F:117:ARG:HH21	2.18	0.42
1:C:35:ILE:O	1:C:39:VAL:HG22	2.19	0.41
1:E:16:VAL:HG12	1:E:27:GLU:HB2	2.02	0.41
1:C:50:MSE:HE1	2:D:58:ALA:O	2.20	0.41
1:G:52:ALA:HB1	2:H:15:ALA:HB2	2.01	0.41
1:E:20:ALA:HB1	1:E:25:VAL:O	2.20	0.41
2:D:-1:SER:C	2:D:0:HIS:CG	2.93	0.41
1:G:59:ARG:HH11	2:H:18:ASP:CG	2.23	0.41
1:G:31:ILE:O	1:G:35:ILE:HG12	2.21	0.41
1:C:23:ARG:HA	2:H:72:ASN:OD1	2.21	0.40
2:B:80:GLN:HE21	2:B:106:ARG:HH22	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
1	C	68/71 (96%)	65 (96%)	3 (4%)	0	100	100
1	E	59/71 (83%)	55 (93%)	4 (7%)	0	100	100
1	G	59/71 (83%)	57 (97%)	2 (3%)	0	100	100
2	B	135/155 (87%)	130 (96%)	5 (4%)	0	100	100
2	D	135/155 (87%)	130 (96%)	5 (4%)	0	100	100
2	F	135/155 (87%)	131 (97%)	4 (3%)	0	100	100
2	H	135/155 (87%)	128 (95%)	7 (5%)	0	100	100
All	All	794/904 (88%)	762 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	51/50 (102%)	50 (98%)	1 (2%)	55	73
1	C	51/50 (102%)	51 (100%)	0	100	100
1	E	45/50 (90%)	44 (98%)	1 (2%)	52	70
1	G	45/50 (90%)	42 (93%)	3 (7%)	16	25
2	B	105/118 (89%)	103 (98%)	2 (2%)	57	74
2	D	105/118 (89%)	104 (99%)	1 (1%)	76	86
2	F	105/118 (89%)	100 (95%)	5 (5%)	25	39
2	H	105/118 (89%)	102 (97%)	3 (3%)	42	60
All	All	612/672 (91%)	596 (97%)	16 (3%)	46	64

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	E	1	MSE
1	G	6	VAL
1	G	12	LEU
1	G	29	GLN
2	B	-1	SER
2	B	120	PHE
2	D	-1	SER
2	F	-1	SER
2	F	105	ASP
2	F	116	ASP
2	F	118	ARG
2	F	119	HIS
2	H	-1	SER
2	H	72	ASN
2	H	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	0	HIS
2	H	72	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	68/71 (95%)	-0.40	0 100 100	35, 56, 81, 95	0
1	C	68/71 (95%)	-0.18	2 (2%) 51 48	42, 60, 89, 128	0
1	E	59/71 (83%)	0.39	7 (11%) 4 3	38, 75, 106, 153	0
1	G	59/71 (83%)	0.22	6 (10%) 6 4	47, 75, 118, 125	0
2	B	136/155 (87%)	-0.37	0 100 100	29, 44, 65, 75	0
2	D	136/155 (87%)	-0.02	4 (2%) 51 48	38, 56, 83, 90	0
2	F	136/155 (87%)	0.16	8 (5%) 22 19	36, 59, 98, 118	0
2	H	136/155 (87%)	-0.19	1 (0%) 87 87	35, 54, 85, 106	0
All	All	798/904 (88%)	-0.08	28 (3%) 44 40	29, 56, 97, 153	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	2	ASP	5.8
1	C	2	ASP	4.8
1	E	2	ASP	4.6
1	E	61	VAL	4.1
1	G	41	GLY	4.0
2	F	118	ARG	3.8
1	G	42	ALA	3.3
2	D	40	VAL	2.9
1	G	61	VAL	2.8
2	F	38	TYR	2.8
1	E	3	LYS	2.8
2	F	110	ARG	2.7
1	E	12	LEU	2.7
1	C	42	ALA	2.6
2	F	-1	SER	2.5
2	H	92	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	39	VAL	2.5
2	D	41	ALA	2.4
1	G	60	ARG	2.3
1	E	60	ARG	2.3
2	F	36	SER	2.2
2	F	108	ARG	2.2
2	D	108	ARG	2.2
2	F	130	ARG	2.1
2	F	30	ALA	2.1
1	E	5	THR	2.1
1	E	55	GLU	2.0
1	G	3	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	H	201	1/1	0.96	0.46	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.